

A DPG-based time-marching scheme for linear hyperbolic problems

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Abstract

The Discontinuous Petrov-Galerkin (DPG) method is a widely employed discretization method for Partial Differential Equations (PDEs). In a recent work, we applied the DPG method with optimal test functions for the time integration of transient parabolic PDEs. We showed that the resulting DPG-based time-marching scheme is equivalent to exponential integrators for the trace variables. In this work, we extend the aforementioned method to time-dependent hyperbolic PDEs. For that, we reduce the second order system in time to first order and we calculate the optimal testing analytically. We also relate our method with exponential integrators of Gautschi-type. Finally, we validate our method for 1D/2D + time linear wave equation after semidiscretization in space with a standard Bubnov-Galerkin method. The presented DPG-based time integrator provides expressions for the solution in the element interiors in addition to those on the traces. This allows to design different error estimators to perform adaptivity.

Keywords: DPG method, Ultraweak variational formulation, Optimal test functions, Exponential integrators, Linear hyperbolic problems, ODE systems

1. Introduction

The Discontinuous Petrov-Galerkin (DPG) method with optimal test functions was introduced by Demkowicz and Gopalakrishnan in 2010 [11, 13]. The main idea of this method is to select optimal test functions that guarantee the discrete stability of non-coercive problems. For that, they proposed to employ test functions that realize the supremum in the inf-sup condition. In general, it is impossible to calculate those optimal test functions exactly (ideal DPG). Therefore, we usually approximate them using a Bubnov-Galerkin method with enriched test spaces (practical DPG). In the last decade, the DPG method [14, 15, 25] has been applied to many problems [9, 10, 12, 16, 18, 19, 21, 38], mostly in frequency domain.

There exist previous works on transient PDEs where the DPG method is applied to the whole space-time domain [17, 20, 22, 26]. This approach allows local space-time refinements but is incompatible with time-stepping. In [23], authors applied the DPG method in space

for the heat equation together with the backward Euler method in time. Recently, in [35], we followed a third approach: to apply the DPG method only in the time variable. In this way, we obtained a DPG-based time-marching scheme for linear transient parabolic PDEs that is compatible with standard Finite Element Method (FEM) based on Bubnov-Galerkin for the space variable.

In this article, we extend our previous work [35] to linear hyperbolic PDEs. First, we consider a single second-order linear Ordinary Differential Equation (ODE). We reduce it to a first order system of the form $U'(t) + AU(t) = F(t)$ by introducing the velocity variable. Then, we consider an ultraweak variational formulation and we calculate the optimal test functions analytically. In this case, it is possible to attain the ideal DPG method because it is a 1D problem and we employ the adjoint norm for the optimal testing. Moreover, with this particular variational setting, the ideal DPG method is equivalent to the optimal testing introduced by Barret and Morton [7] in the 80's. The optimal test functions we obtain are exponentials of the matrix A that solve the adjoint problem. Finally, we substitute the optimal test functions into the ultraweak variational formulation and we obtain the DPG-based time-marching scheme. Here, we obtain an independent formula for the trace variables and a system to locally compute the interiors of the elements. The generalization to a system of ODEs coming from the spatial discretization of a hyperbolic PDE is straightforward.

The main benefit of the presented method is that it fits into the DPG theory. Therefore, we can naturally apply adaptive strategies and a posteriori error estimation previously studied by the DPG community. Currently, most of the goal-oriented adaptive strategies for transient problems are based on Discontinuous-Galerkin (DG) formulations in time [6] because we need a variational formulation in time to represent the error in the quantity of interest over the whole space-time domain. Employing the variational formulation presented in this article, we will be able to design goal-oriented adaptive strategies in the future based on the DPG method both in space and time.

As we showed in [35], the equation we obtain for the trace variables is called variation-of-constants formula and it is the starting point of exponential integrators [30, 32]. Different approximations of this formula lead to different methods [31, 33, 34]. In all of them, it is necessary to approximate the exponential of a matrix and related functions called φ -functions. For the hyperbolic case, there exist an alternative approach that uses the ideas introduced by Gautschi [24] in the early 60's. As the matrix A is anti-diagonal, we can apply the Cayley-Hamilton theorem and express the system in terms of trigonometric functions [4, 5, 36]. Although the theory of exponential integrators is classical, they have recently gained popularity due to the rise of the available software and efficient algorithms to compute the action of function matrices over vectors. There exist an extensive literature and software to efficiently compute approximation of functions of matrices: exponential, φ -functions, trigonometric functions, etc. See Higham et. al [28] and references therein.

In this work, we relate our DPG-based time-marching scheme with both exponential integrator approaches for hyperbolic problems: In the first one, we express the optimal test functions from DPG in terms of φ -functions. Therefore, we obtain a classical exponential integrator to compute the trace variables, and we compute the interiors of the elements.

The second approach expresses the DPG method in terms of trigonometric functions using the Cayley-Hamilton theorem, and we obtain Gautschi-type methods for the trace variables. The calculation of the optimal test functions and their relation with the φ -functions is the same as in parabolic problems. Nevertheless, the reduction to a first order system and the relation of the DPG method with trigonometric functions is a new contribution comparing with the parabolic case. In the numerical results of this article, we validate both approaches. We employ three MATLAB routines: the two ones in [8, 27] for computing φ -functions based on a scaling and squaring algorithm together with Padé approximations; and the one in [1] based on a truncated Taylor series to approximate trigonometric functions. We also discuss the main implementation difficulties encountered in the hyperbolic case that are not present in parabolic problems. In the hyperbolic case, the system matrix is double size comparing to the parabolic problem, which leads to memory limitations. Finally, we observe that many iterative methods that are efficient for parabolic problems do not converge for the wave equation at high frequencies.

This work is organized as follows: Section 2 states the variational setting for a single linear second order ODE. Section 3 provides an overview of the ideal DPG method with optimal test functions, we proposed in [35]. We generalize the method in Section 4 for a system of ODEs. Section 5 shows the relation between the proposed DPG method and exponential integrators. Section 6 provides a discussion on the implementation. In Section 7, we present the numerical results for a single ODE, and 1D/2D+time linear wave equation. Section 8 summarizes the conclusions and future research lines. Finally, in Appendix A we provide the Cayley-Hamilton theorem.

2. Variational setting of second order ODEs

Let $I = (0, 1] \subset \mathbb{R}$. We consider the following second order Ordinary Differential Equation (ODE)

$$\begin{cases} u''(t) + \alpha^2 u(t) = f(t) & \text{in } I, \\ u(0) = u_0, \\ u'(0) = v_0, \end{cases} \quad (1)$$

where u'' denotes the second derivative of u , $\alpha^2 \in \mathbb{R} - \{0\}$ and $f \in L^2(I)$. In (1), the source $f(t)$ and the initial conditions $u_0, v_0 \in \mathbb{R}$ are given data.

In order to obtain an ultraweak formulation, we first reduce (1) to a first order system defining $v(t) = u'(t)$

$$\begin{cases} U'(t) + AU(t) = F(t) & \text{in } I, \\ U(0) = U_0, \end{cases} \quad (2)$$

where

$$U(t) = \begin{bmatrix} u(t) \\ v(t) \end{bmatrix}, \quad A = \begin{bmatrix} 0 & -1 \\ \alpha^2 & 0 \end{bmatrix}, \quad F(t) = \begin{bmatrix} 0 \\ f(t) \end{bmatrix}, \quad U_0 = \begin{bmatrix} u_0 \\ v_0 \end{bmatrix}.$$

We denote by (\cdot, \cdot) the usual dot product in \mathbb{R}^n where $(U, W) = U^T \cdot W$ and $\|\cdot\|$ the Euclidean norm of \mathbb{R}^n so $\|\cdot\|^2 = (\cdot, \cdot)$. We now multiply the equation (2) by some suitable

test functions $W(t) = \begin{bmatrix} w(t) \\ \sigma(t) \end{bmatrix}$ and we integrate over I

$$\int_I (U' + AU, W) dt = \int_I (F, W) dt.$$

Integrating by parts in time and employing that $(AU, W) = (U, A^T W)$, we obtain

$$\int_I (U, -W' + A^T W) dt + (U(1), W(1)) - (U(0), W(0)) = \int_I (F, W) dt.$$

We substitute $U(0)$ by U_0 and we consider the unknown $U(1)$ as a separate variable that we denote $\hat{U} = \begin{bmatrix} \hat{u} \\ \hat{v} \end{bmatrix}$. Finally, we obtain the following ultraweak variational formulation of problem (2)

$$\begin{cases} \text{Find } Z = \{U, \hat{U}\} \in \mathcal{U} \text{ such that} \\ \mathcal{B}(Z, W) = \mathcal{L}(W), \quad \forall W \in \mathcal{W}, \end{cases} \quad (3)$$

where

$$\begin{aligned} \mathcal{B}(Z, W) &:= \int_I (U, -W' + A^T W) dt + (\hat{U}, W(1)), \\ \mathcal{L}(W) &:= \int_I (F, W) dt + (U_0, W(0)). \end{aligned}$$

The trial and test spaces are $\mathcal{U} = \mathcal{U}_0 \times \hat{\mathcal{U}} := L^2(I, \mathbb{R}^2) \times \mathbb{R}^2$ and $\mathcal{W} = H^1(I, \mathbb{R}^2)$, with the following norms

$$\begin{aligned} \|Z\|_{\mathcal{U}}^2 &= \int_I \|U\|^2 dt + \|\hat{U}\|^2, \\ \|W\|_{\mathcal{W}}^2 &= \int_I \|-W' + A^T W\|^2 dt + \|W(1)\|^2. \end{aligned} \quad (4)$$

Formulation (3) is equivalent to the following problem

$$\begin{cases} \text{Find } \{u, \hat{u}\} \in L^2(I) \times \mathbb{R}, \{v, \hat{v}\} \in L^2(I) \times \mathbb{R} \text{ such that} \\ - \int_I u w' dt + \hat{u} w(1) - \int_I v w dt = u_0 w(0), \quad \forall w \in H^1(I), \\ - \int_I v \sigma' dt + \hat{v} \sigma(1) + \alpha^2 \int_I u \sigma dt = \int_I f \sigma dt + v_0 \sigma(0), \quad \forall \sigma \in H^1(I). \end{cases}$$

3. Overview of the ideal DPG method with optimal test functions

This section provides an overview of the ideal DPG method and how to calculate the optimal test functions for a system of the form (2). More details on this part are explained in [35].

3.1. Optimal test functions over a single element

Given a discrete subspace $\mathcal{U}_h = \mathcal{U}_{h,0} \times \hat{\mathcal{U}} \subset \mathcal{U}$, we introduce the following *ideal Petrov-Galerkin (PG) method* as

$$\begin{cases} \text{Find } Z_h = \{U_h, \hat{U}_h\} \in \mathcal{U}_{h,0} \times \hat{\mathcal{U}} \text{ such that} \\ \mathcal{B}(Z_h, W_h) = \mathcal{L}(W_h), \quad \forall W_h \in \mathcal{W}_h^{opt}, \end{cases} \quad (5)$$

where \mathcal{W}_h^{opt} is called the *optimal test space* for the continuous bilinear form $\mathcal{B}(\cdot, \cdot)$. We introduce the *trial-to-test operator* $\Phi : \mathcal{U}_h \rightarrow \mathcal{W}$ by

$$(\Phi Z_h, \delta W)_{\mathcal{W}} = \mathcal{B}(Z_h, \delta W), \quad \forall \delta W \in \mathcal{W}, \quad Z_h \in \mathcal{U}_h, \quad (6)$$

being $(\cdot, \cdot)_{\mathcal{W}}$ an inner product in \mathcal{W} . Then, the optimal test space is defined by $\mathcal{W}_h^{opt} := \Phi(\mathcal{U}_h)$ and, from (6), we establish it has the same dimension as \mathcal{U}_h .

Remark 1. We know from [14] that the solution Z_h of the ideal PG method (5) is unique and it holds

$$\|Z - Z_h\|_{\mathcal{U}} \leq \frac{M}{\gamma} \inf_{X_h \in \mathcal{U}_h} \|Z - X_h\|_{\mathcal{U}},$$

where Z is the exact solution of (3). Moreover, $M = \gamma = 1$ with respect the norms defined in (4). It also holds that Z_h is the best approximation to Z

$$\|Z - Z_h\|_E = \inf_{X_h \in \mathcal{U}_h} \|Z - X_h\|_E,$$

in the energy norm defined by $\|Z\|_E := \sup_{0 \neq W \in \mathcal{W}} \frac{|\mathcal{B}(Z, W)|}{\|W\|_{\mathcal{W}}}$.

In [35], we calculate the optimal test functions analytically by solving (6). Given a trial function $Z_h = \{U_h, \hat{U}_h\} \in \mathcal{U}_h$, we find $\mathbf{W} := \Phi Z_h \in \mathcal{W}$ satisfying (6), which is equivalent to the following Boundary Value Problem (BVP)

$$\begin{cases} -\mathbf{W}' + A^T \mathbf{W} = U_h, \\ \mathbf{W}(1) = \hat{U}_h. \end{cases} \quad (7)$$

The solution of (7) is

$$\Phi Z_h = \Phi\{U_h, \hat{U}_h\} = e^{A^T(t-1)}\hat{U}_h + \int_t^1 e^{A^T(t-\tau)}U_h(\tau)d\tau. \quad (8)$$

We select in (5) a trial space $\mathcal{U}_{h,0}$ of piecewise polynomials of order p . Then, we express the interiors of the solution $Z_h = \{U_h, \hat{U}_h\} \in \mathcal{U}_h$ as

$$U_h(t) = \sum_{j=0}^p U_{h,j} t^j, \quad U_{h,j} = \begin{bmatrix} u_{h,j} \\ v_{h,j} \end{bmatrix} \in \mathbb{R}^2, \quad \forall j = 0, \dots, p.$$

We denote by $\{\mathbf{e}_1, \mathbf{e}_2\}$ the canonical basis of \mathbb{R}^2 and $\mathbf{0} \in \mathbb{R}^2$ the zero vector. Therefore, $\mathcal{U}_{h,0} = \text{span}\{\mathbf{e}_1 t^j, \mathbf{e}_2 t^j, j = 0, \dots, p\}$ and $\hat{\mathcal{U}} = \text{span}\{\mathbf{e}_1, \mathbf{e}_2\}$. Now, we calculate the optimal test functions corresponding to \mathcal{U}_h employing the trial-to-test operator (8).

The optimal test functions corresponding to the trace variables are

$$\hat{\mathbf{W}}_i(A^T, t) := \Phi\{\mathbf{0}, \mathbf{e}_i\} = e^{A^T(t-1)} \mathbf{e}_i, \quad \forall i = 1, 2, \quad (9)$$

and we calculate the optimal test functions corresponding to the interiors recursively as

$$\begin{aligned} \mathbf{W}_{r,i}(A^T, t) &:= \Phi\{t^r \mathbf{e}_i, \mathbf{0}\} = \int_t^1 e^{A^T(t-\tau)} \tau^r \mathbf{e}_i d\tau \\ &= (A^T)^{-1} \left(t^r I_n - e^{A^T(t-1)} + r \int_t^1 e^{A^T(t-\tau)} \tau^{r-1} d\tau \right) \mathbf{e}_i, \\ &= (A^T)^{-1} \left(t^p \mathbf{e}_i + p \mathbf{W}_{p-1,i}(A^T, t) - \hat{\mathbf{W}}_i(A^T, t) \right) \end{aligned} \quad (10)$$

$\forall r = 0, \dots, p, \forall i = 1, 2$. From (7), these functions satisfy

$$\begin{aligned} -\hat{\mathbf{W}}'_i(A^T, t) + A^T \hat{\mathbf{W}}_i(A^T, t) &= \mathbf{0}, \quad \mathbf{W}_{p,i}(A^T, 1) = \mathbf{e}_i, \quad \forall i = 1, 2, \\ -\mathbf{W}'_{r,i}(A^T, t) + A^T \mathbf{W}_{r,i}(A^T, t) &= t^r \mathbf{e}_i, \quad \mathbf{W}_{r,i}(A^T, 1) = \mathbf{0}, \quad \forall i = 1, 2. \end{aligned} \quad (11)$$

Therefore, the optimal test space in (5) is $\mathcal{W}_h^{opt} = \text{span}\{\hat{\mathbf{W}}_i, \mathbf{W}_{r,i}, \forall r = 0, \dots, p, \forall i = 1, 2\}$ and we obtain the following scheme for problem (5)

$$\left\{ \begin{aligned} (\hat{U}_h, \mathbf{e}_i) &= (U_0, \hat{\mathbf{W}}_i(A^T, 0)) + \int_0^1 (F(t), \hat{\mathbf{W}}_i(A^T, t)) dt, \quad \forall i = 1, 2, \\ \int_0^1 \left(\sum_{j=0}^p U_{h,j} t^j, t^r \mathbf{e}_i \right) dt &= (U_0, \mathbf{W}_{r,i}(A^T, 0)) + \int_0^1 (F(t), \mathbf{W}_{r,i}(A^T, t)) dt, \\ &\quad \forall r = 0, \dots, p, \forall i = 1, 2. \end{aligned} \right. \quad (12)$$

We express (12) in matrix form as

$$\left\{ \begin{aligned} \hat{U}_h^T &= U_0^T \cdot \hat{\mathbf{W}}(A^T, 0) + \int_0^1 F^T(t) \cdot \hat{\mathbf{W}}(A^T, t) dt, \\ \sum_{j=0}^p U_{h,j}^T \int_0^1 t^{j+r} dt &= U_0^T \cdot \mathbf{W}_r(A^T, 0) + \int_0^1 F^T(t) \cdot \mathbf{W}_r(A^T, t) dt, \quad \forall r = 0, \dots, p, \end{aligned} \right. \quad (13)$$

where $\hat{\mathbf{W}}(A^T, t) = e^{A^T(t-1)}$ and

$$\mathbf{W}_r(A^T, t) = (A^T)^{-1} \left(t^r I_2 + r \mathbf{W}_{r-1}(A^T, t) - \hat{\mathbf{W}}(A^T, t) \right), \quad \forall r = 0, \dots, p. \quad (14)$$

In [35], we also proved that the optimal test functions satisfy

$$\mathbf{W}_r(A^T, t) = (A^T)^{-r-1} \left(\mathcal{P}_r(A^T, t) - \mathcal{P}_r(A^T, 1) \hat{\mathbf{W}}(A^T, t) \right), \quad \forall r = 0, \dots, p. \quad (15)$$

where $\mathcal{P}_p(A^T, t)$ is a polynomial of order p defined as

$$\mathcal{P}_p(A^T, t) = \sum_{j=0}^p \frac{p!}{j!} (A^T t)^j.$$

Finally, if we transpose the whole system (13), as

$$(\hat{\mathbf{W}}(A^T, t))^T = \hat{\mathbf{W}}(A, t), \quad (\mathbf{W}_r(A^T, t))^T = \mathbf{W}_r(A, t), \quad \forall r = 0, \dots, p,$$

we obtain

$$\begin{cases} \hat{U}_h = \hat{\mathbf{W}}(A, 0) \cdot U_0 + \int_0^1 \hat{\mathbf{W}}(A, t) \cdot F(t) dt, \\ \sum_{j=0}^p U_{h,j} \int_0^1 t^{j+r} dt = \mathbf{W}_r(A, 0) \cdot U_0 + \int_0^1 \mathbf{W}_r(A, t) \cdot F(t) dt, \quad \forall r = 0, \dots, p. \end{cases} \quad (16)$$

3.2. Extension to a general number of elements

We consider a partition of the time interval I_h as

$$0 = t_0 < t_1 < \dots < t_{m-1} < t_m = 1, \quad (17)$$

and we define $I_k = (t_{k-1}, t_k)$ and the time step size $h_k = t_k - t_{k-1}$, $\forall k = 1, \dots, m$. We now repeat the same process of Subsection 3.1 over a generic element I_k . First, we express the interior and the traces of the approximated solution $U_h(t)$ over the generic element I_k as

$$U_h^k(t) = \sum_{j=0}^p U_{h,j}^k \left(\frac{t - t_{k-1}}{h_k} \right)^j, \quad U_{h,j}^k = \begin{bmatrix} u_{h,j}^k \\ v_{h,j}^k \end{bmatrix}, \quad \hat{U}_h^k = \begin{bmatrix} \hat{u}_h^k \\ \hat{v}_h^k \end{bmatrix}.$$

The optimal test functions are $\hat{\mathbf{W}}^k(A^T, t) = e^{A^T(t-t_k)}$, and

$$\begin{aligned} \mathbf{W}_r^k(A^T, t) &= (A^T)^{-1} \left(\left(\frac{t - t_{k-1}}{h_k} \right)^r I_2 + \frac{r}{h_k} \mathbf{W}_{r-1}^k(A^T, t) - \hat{\mathbf{W}}^k(A^T, t) \right) \\ &= \frac{1}{h_k^r} (A^T)^{-r-1} \left(\mathcal{P}_r^k(A^T, t) - \mathcal{P}_r^k(A^T, t_k) \hat{\mathbf{W}}^k(A^T, t) \right), \end{aligned} \quad (18)$$

where $\mathcal{P}_r^k(A^T, t)$ is defined as

$$\mathcal{P}_r^k(A^T, t) = \sum_{j=0}^r \frac{r!}{j!} (A^T)^j (t - t_{k-1})^j.$$

Here, the optimal test functions (18) satisfy

$$\begin{cases} -(\hat{\mathbf{W}}^k(A^T, t))' + A^T \hat{\mathbf{W}}^k(A^T, t) = \mathbf{0}, & \hat{\mathbf{W}}^k(A^T, t_k) = I_2, \\ -(\mathbf{W}_r^k(A^T, t))' + A^T \mathbf{W}_r^k(A^T, t) = \left(\frac{t - t_{k-1}}{h_k} \right)^r I_2, & \mathbf{W}_r^k(A^T, t_k) = \mathbf{0}, \quad \forall r = 0, \dots, p, \end{cases}$$

and we obtain the following time-marching scheme $\forall k = 1, \dots, m$

$$\begin{cases} \hat{U}_h^k = \hat{\mathbf{W}}^k(A, t_{k-1}) \cdot \hat{U}_h^{k-1} + \int_{I_k} \hat{\mathbf{W}}^k(A, t) \cdot F(t) dt, \\ \sum_{j=0}^p U_{h,j}^k \int_{I_k} \left(\frac{t - t_{k-1}}{h_k} \right)^{j+r} dt = \mathbf{W}_r^k(A, t_{k-1}) \cdot \hat{U}_h^{k-1} + \int_{I_k} \mathbf{W}_r^k(A, t) \cdot F(t) dt, \quad \forall r = 0, \dots, p, \end{cases} \quad (19)$$

where $\hat{U}_h^0 = U_0$. Therefore, computing the optimal test functions over one element I_k , we obtain scheme (19). Here, we know \hat{U}_h^{k-1} which is the solution at t_{k-1} . Then, we employ the second equation of (19) to compute the interior of the solution at I_k and the first equation of (19) to calculate the solution at t_k , i.e., \hat{U}_h^k . Finally, the trace solution \hat{U}_h^k becomes the initial condition for the next interval.

Remark 2. As an alternative to Section 3.2, we can express the optimal testing problem (6) globally by introducing a broken test space. In [35], we proved that the optimal test space we obtain from the broken formulation is the span of the optimal test functions defined in (18). Therefore, both approaches deliver the same solution.

4. Application to linear ODE systems

We now consider the following linear system of ODEs

$$\begin{cases} u''(t) + Cu(t) = f(t), & \text{in } I, \\ u(0) = u_0, \\ v(0) = v_0, \end{cases} \quad (20)$$

where $C \in \mathbb{R}^{n \times n}$, $u_0, v_0 \in \mathbb{R}^n$ and $u, f : I \rightarrow \mathbb{R}^n$

$$u(t) = \begin{bmatrix} u_1(t) \\ \vdots \\ u_n(t) \end{bmatrix}, \quad f(t) = \begin{bmatrix} f_1(t) \\ \vdots \\ f_n(t) \end{bmatrix}, \quad u_0 = \begin{bmatrix} u_{0,1} \\ \vdots \\ u_{0,n} \end{bmatrix}, \quad v_0 = \begin{bmatrix} v_{0,1} \\ \vdots \\ v_{0,n} \end{bmatrix}.$$

We are interested in the particular case where C is a matrix resulting from a spatial discretization of a linear hyperbolic PDE.

As in Section 2, we reduce (20) to a first order system by defining $v(t) = u'(t)$ so we have

$$\begin{cases} U'(t) + AU(t) = F(t) & \text{in } I, \\ U(0) = U_0, \end{cases} \quad (21)$$

where

$$U(t) = \begin{bmatrix} u(t) \\ v(t) \end{bmatrix}, \quad A = \begin{bmatrix} 0 & -I_n \\ C & 0 \end{bmatrix}, \quad F(t) = \begin{bmatrix} 0 \\ f(t) \end{bmatrix}, \quad U_0 = \begin{bmatrix} u_0 \\ v_0 \end{bmatrix}.$$

Here, 0 denotes the zero matrix or vector of appropriate size, $U, F : I \rightarrow \mathbb{R}^{2n}$, $U_0 \in \mathbb{R}^{2n}$ and $A \in \mathbb{R}^{2n \times 2n}$. The application of the DPG method defined in Section 3 to system (21) is straightforward.

5. Relation between ideal DPG method and exponential integrators

Exponential integrators are a class of well-established methods for solving semilinear systems of ODEs [32]. The starting point of many exponential integrators is the fact that the analytical solution of system (2) can be expressed by the variation-of-constants formula

$$U(t) = e^{-At}U_0 + \int_0^t e^{A(\tau-t)}F(\tau)d\tau. \quad (22)$$

From (22), we can express the solution at each time step as

$$U(t_k) = e^{-h_k A}U(t_{k-1}) + \int_{I_k} e^{A(\tau-t_k)}F(\tau)d\tau, \quad (23)$$

and different approximations of the right-hand-side of (23) lead to different methods. In the DPG-based time-marching scheme (19), as $\hat{\mathbf{W}}^k(A, t) = e^{A(t-t_k)}$, we have the variation-of-constants formula (23) for the trace variables. Therefore, the DPG method in time is equivalent to exponential integrators for the traces and we have an additional equation to compute the interiors of the solution. In the following subsections, we explain how to approximate (19) employing the ideas from exponential integrators.

5.1. φ -functions

Similar to our previous work for parabolic problems [35], we can approximate the right-hand-side of system (19) with exponential quadrature rules and so-called φ -functions. First, we select s integration points $c_i \in [0, 1]$, $\forall i = 1, \dots, s$ and we approximate the source at each element I_k as

$$F(t)|_{I_k} \approx \sum_{i=1}^s F_i^k L_i^k(t),$$

where $F_i := F(t_{k-1} + c_i h_k)$ and $L_i^k(t)$ are the Legendre polynomials at I_k defined as

$$L_i^k(t) = \prod_{\substack{j=1 \\ j \neq i}}^s \frac{t - (t_{k-1} + c_j h_k)}{(t_{k-1} + c_i h_k) - (t_{k-1} + c_j h_k)}, \quad \forall i = 1, \dots, s.$$

Then, (19) becomes

$$\left\{ \begin{array}{l} \hat{U}_h^k = \hat{\mathbf{W}}^k(A, t_{k-1}) \cdot \hat{U}_h^{k-1} + \sum_{i=1}^s \left(\int_{I_k} \hat{\mathbf{W}}^k(A, t) L_i^k(t) dt \right) \cdot F_i, \\ \sum_{j=0}^p U_{h,j}^k \int_{I_k} \left(\frac{t - t_{k-1}}{h_k} \right)^{j+r} dt = \mathbf{W}_r^k(A, t_{k-1}) \cdot \hat{U}_h^{k-1} + \sum_{i=1}^s \left(\int_{I_k} \mathbf{W}_r^k(A, t) L_i^k(t) dt \right) \cdot F_i, \\ \forall r = 0, \dots, p. \end{array} \right. \quad (24)$$

The optimal test functions satisfy the following identities

$$\begin{aligned}\hat{\mathbf{W}}^k(A, t_{k-1} + \theta h_k) &= \hat{\mathbf{W}}(Ah_k, \theta), \\ \mathbf{W}_r^k(A, t_{k-1} + \theta h_k) &= h_k \mathbf{W}_r(Ah_k, \theta), \quad \forall r = 0, \dots, p,\end{aligned}$$

where $\hat{\mathbf{W}}(A, t)$ and $\mathbf{W}_r(A, t)$ are the optimal test functions defined over the master element $[0, 1]$. We now express (24) over $[0, 1]$ and we obtain

$$\left\{ \begin{aligned} \hat{U}_h^k &= \hat{\mathbf{W}}(Ah_k, 0) \cdot \hat{U}_h^{k-1} + h_k \sum_{i=1}^s \left(\int_0^1 \hat{\mathbf{W}}(Ah_k, \theta) L_i(\theta) d\theta \right) \cdot F_i, \\ h_k \sum_{j=0}^p U_{h,j}^k \int_0^1 \theta^{j+r} d\theta &= h_k \mathbf{W}_r(Ah_k, 0) \cdot \hat{U}_h^{k-1} + h_k \sum_{i=1}^s \left(\int_0^1 h_k \mathbf{W}_r(Ah_k, \theta) L_i(\theta) d\theta \right) \cdot F_i, \\ \forall r &= 0, \dots, p, \end{aligned} \right. \quad (25)$$

where $L_i(\theta)$ are the Legendre polynomials defined over $[0, 1]$.

Finally, integrating the left-hand-side of (25) and simplifying h_k from the second equation, we obtain

$$\left\{ \begin{aligned} \hat{U}_h^k &= \hat{\mathbf{W}}(Ah_k, 0) \cdot \hat{U}_h^{k-1} + h_k \sum_{i=1}^s \left(\int_0^1 \hat{\mathbf{W}}(Ah_k, \theta) L_i(\theta) d\theta \right) \cdot F_i, \\ \sum_{j=0}^p U_{h,j}^k \frac{1}{j+r+1} &= \mathbf{W}_r(Ah_k, 0) \cdot \hat{U}_h^{k-1} + h_k \sum_{i=1}^s \left(\int_0^1 \mathbf{W}_r(Ah_k, \theta) L_i(\theta) d\theta \right) \cdot F_i, \\ \forall r &= 0, \dots, p. \end{aligned} \right. \quad (26)$$

In (26), we relate the optimal test functions with the so-called φ -functions defined as

$$\left\{ \begin{aligned} \varphi_0(A) &= e^A, \\ \varphi_p(A) &= \int_0^1 e^{(1-\theta)A} \frac{\theta^{p-1}}{(p-1)!} d\theta, \quad \forall p \geq 1, \end{aligned} \right. \quad (27)$$

which satisfy the following recurrence relation

$$\varphi_p(A) = \frac{1}{p!} I_n + A \varphi_{p+1}(A), \quad (28)$$

where I_n denotes the identity matrix in \mathbb{R}^n . Note that $\varphi_p(A)$ is another matrix of size $n \times n$.

In [35], we proved that

$$\hat{\mathbf{W}}(A, 0) = e^{-A} = \varphi_0(-A), \quad (29a)$$

$$\int_0^1 \hat{\mathbf{W}}(A, \theta) \theta^q d\theta = \int_0^1 e^{A(\theta-1)} \theta^q d\theta = q! \varphi_{q+1}(-A), \quad (29b)$$

and also

$$\mathbf{W}_r(A, 0) = \sum_{j=0}^r \frac{r!}{j!} (-1)^{r-j} \varphi_{r-j+1}(-A), \quad (30a)$$

$$\int_0^1 \mathbf{W}_r(A, \theta) \theta^q d\theta = q! \sum_{j=0}^r \frac{r!}{j!} (-1)^{r-j} \varphi_{r-j+q+2}(-A). \quad (30b)$$

Therefore, we can express $L_i(\theta)$ as linear combinations of polynomials of type θ^q and then use (29) and (30) to express (26) in terms of the φ -functions.

5.2. Trigonometric functions

In hyperbolic systems of type (2) or (21), from the reduction to a first order system, the matrix A is always anti-diagonal. Therefore, we can calculate its eigenvalues and apply the Cayley-Hamilton theorem (see Appendix A). For simplicity, we focus on system (2) where the matrix A has complex eigenvalues $\pm i\alpha$. From the Cayley-Hamilton theorem, we have

$$e^{At} = \begin{bmatrix} \cos(\alpha t) & -\frac{1}{\alpha} \sin(\alpha t) \\ \alpha \sin(\alpha t) & \cos(\alpha t) \end{bmatrix}. \quad (31)$$

Now, in (19) we obtain

$$\hat{\mathbf{W}}^k(A, t) = e^{A(t-t_k)} = \begin{bmatrix} \cos(\alpha(t-t_k)) & -\frac{1}{\alpha} \sin(\alpha(t-t_k)) \\ \alpha \sin(\alpha(t-t_k)) & \cos(\alpha(t-t_k)) \end{bmatrix}, \quad (32)$$

$$\hat{\mathbf{W}}^k(A, t_{k-1}) = e^{-Ah_k} = \begin{bmatrix} \cos(\alpha h_k) & \frac{1}{\alpha} \sin(\alpha h_k) \\ -\alpha \sin(\alpha h_k) & \cos(\alpha h_k) \end{bmatrix}, \quad (33)$$

and the equation for the trace variables in (19) becomes

$$\begin{bmatrix} \hat{u}_h^k \\ \hat{v}_h^k \end{bmatrix} = \begin{bmatrix} \cos(\alpha h_k) & \frac{1}{\alpha} \sin(\alpha h_k) \\ -\alpha \sin(\alpha h_k) & \cos(\alpha h_k) \end{bmatrix} \begin{bmatrix} \hat{u}_h^{k-1} \\ \hat{v}_h^{k-1} \end{bmatrix} + \int_{I_k} \begin{bmatrix} -\frac{1}{\alpha} \sin(\alpha(t-t_k)) \\ \cos(\alpha(t-t_k)) \end{bmatrix} f(t) dt.$$

Similarly for the second equation of (19), we express $\mathbf{W}_r^k(A, t)$ and $\mathbf{W}_r^k(A, t_{k-1})$ in terms of (32) and (33) employing relation (18). Finally, we approximate the right-hand-side of (19) approximating $f(t)$ and integrating exactly.

Example: For $p = 0$ and approximating $f(t) \approx f(t_{k-1})$, the first equation of system (19) becomes

$$\begin{bmatrix} \hat{u}_h^k \\ \hat{v}_h^k \end{bmatrix} = \begin{bmatrix} \cos(\alpha h_k) & \frac{1}{\alpha} \sin(\alpha h_k) \\ -\alpha \sin(\alpha h_k) & \cos(\alpha h_k) \end{bmatrix} \begin{bmatrix} \hat{u}_h^{k-1} \\ \hat{v}_h^{k-1} \end{bmatrix} + \begin{bmatrix} \frac{1}{\alpha^2} (1 - \cos(\alpha h_k)) \\ \frac{1}{\alpha} \sin(\alpha h_k) \end{bmatrix} f(t_{k-1}). \quad (34)$$

From (18), we have

$$\mathbf{W}_0^k(A, t) = A^{-1} \left(I_2 - \hat{\mathbf{W}}^k(A, t) \right) = \begin{bmatrix} -\frac{1}{\alpha} \sin(\alpha(t-t_k)) & \frac{1}{\alpha^2} (1 - \cos(\alpha(t-t_k))) \\ \cos(\alpha(t-t_k)) - 1 & -\frac{1}{\alpha} \sin(\alpha(t-t_k)) \end{bmatrix},$$

$$\mathbf{W}_0^k(A, t_{k-1}) = \begin{bmatrix} \frac{1}{\alpha} \sin(\alpha h_k) & \frac{1}{\alpha^2} (1 - \cos(\alpha h_k)) \\ \cos(\alpha h_k) - 1 & \frac{1}{\alpha} \sin(\alpha h_k) \end{bmatrix},$$

and the second equation of (19) becomes

$$h_k \begin{bmatrix} u_{h,0}^k \\ v_{h,0}^k \end{bmatrix} = \begin{bmatrix} \frac{1}{\alpha} \sin(\alpha h_k) & \frac{1}{\alpha^2} (1 - \cos(\alpha h_k)) \\ \cos(\alpha h_k) - 1 & \frac{1}{\alpha} \sin(\alpha h_k) \end{bmatrix} \begin{bmatrix} \hat{u}_h^{k-1} \\ \hat{v}_h^{k-1} \end{bmatrix} + \begin{bmatrix} \frac{1}{\alpha^3} (\alpha h_k - \sin(\alpha h_k)) \\ \frac{1}{\alpha^2} (1 - \cos(\alpha h_k)) \end{bmatrix} f(t_{k-1}). \quad (35)$$

In exponential integrators, the trigonometric functions are usually given in terms of $\text{sinc}(\xi) = \sin(\xi)/\xi$. Therefore, applying basic trigonometric identities, (34) and (35) become

$$\begin{bmatrix} \hat{u}_h^k \\ \hat{v}_h^k \end{bmatrix} = \begin{bmatrix} \cos(\alpha h_k) & h_k \text{sinc}(\alpha h_k) \\ -\alpha \sin(\alpha h_k) & \cos(\alpha h_k) \end{bmatrix} \begin{bmatrix} \hat{u}_h^{k-1} \\ \hat{v}_h^{k-1} \end{bmatrix} + h_k \begin{bmatrix} \frac{h_k}{2} \text{sinc}^2(\frac{\alpha h_k}{2}) \\ \text{sinc}(\alpha h_k) \end{bmatrix} f(t_{k-1}), \quad (36)$$

$$\begin{bmatrix} u_{h,0}^k \\ v_{h,0}^k \end{bmatrix} = \begin{bmatrix} \text{sinc}(\alpha h_k) & \frac{h_k}{2} \text{sinc}^2(\frac{\alpha h_k}{2}) \\ -\frac{\alpha^2 h_k}{2} \text{sinc}^2(\frac{\alpha h_k}{2}) & \text{sinc}(\alpha h_k) \end{bmatrix} \begin{bmatrix} \hat{u}_h^{k-1} \\ \hat{v}_h^{k-1} \end{bmatrix} + \begin{bmatrix} \frac{1}{\alpha^2} (1 - \text{sinc}(\alpha h_k)) \\ \frac{h_k}{2} \text{sinc}^2(\frac{\alpha h_k}{2}) \end{bmatrix} f(t_{k-1}).$$

The first equation of (36) is called Gautschi method [24].

Remark 3. *The theory presented in this paper is consistent with the case $\alpha = 0$. Note that when $\alpha = 0$, matrix A is nilpotent, i.e., $A^2 = 0$. Therefore, from the series expansion of the exponential we have*

$$e^{At} = I + At = \begin{bmatrix} 1 & -t \\ 0 & 1 \end{bmatrix}. \quad (37)$$

In this case, recurrence relation (18) is not valid because A is a singular matrix. We can calculate the optimal test function explicitly using the trial-to-test operator (8) and (37).

6. Implementation aspects

The crucial and most expensive part in the time-marching schemes presented in this article –(26) and (36)– is the approximation of functions of matrices (exponential, trigonometric functions, and φ –functions). There exist multiple algorithms to compute exponential matrices and related functions (see the recent catalogue by N. J. Highman et al [28]). In this section, we briefly discuss some of the different MATLAB packages we have employed for the numerical results in this work, and the implementation and numerical difficulties we have encountered with respect to the parabolic case in [35].

- The EXPINT package [8] includes a routine to approximate $\varphi_p(A)$, $\forall p \geq 1$ of a given matrix A . The method is based on a scaling and squaring algorithm together with Padé approximations. The routine works properly for the hyperbolic case; however, it becomes inefficient in terms of memory for large problems. The reason is that the matrix A for the hyperbolic case is double size comparing with the parabolic case. Moreover, we need to compute several matrices $\varphi_p(A)$ per time step that are dense matrices even if matrix A is sparse.

- The built-in MATLAB function $\text{expm}()$ [2, 27] approximates the exponential of a matrix $\text{expm}(A) = e^A$. There is a classical result that relates the following action

$$\sum_{j=1}^p \varphi_j(A) w_{p-j+1}, \quad (38)$$

for some vectors $\{w_j\}_{j=1}^p$ with the columns of the exponential of an augmented matrix \tilde{A} (See Theorem 2.1. in [3]). Therefore, in the right-hand-side of (26), we can avoid the approximations of the corresponding φ -functions by computing the single exponential of a slightly larger matrix $\text{expm}(\tilde{A})$. This routine provides adequate results for the hyperbolic case, but it still requires to store a full exponential matrix per time step. The routine defined in [3] by the same authors avoids such storage by approximating the action of the matrix exponential over vectors with truncated Taylor series.

- The *phipm*() routine introduced in [37] is an iterative method based on Krylov subspaces that approximates (38). The entries of the routine are the matrix A and the vectors $\{w_j\}$, and it returns the action (38). In this case, the matrix A is reduced to a smaller one by projecting it onto a Krylov subspace. This algorithm is efficient for parabolic problems and it relaxes the memory limitations. However, this iterative routine does not converge for the wave equation problems at high frequencies considered in this article.
- We have also investigated some recent research (see [1, 4, 5, 36]) to approximate the trigonometric functions of matrices defined in Section 5.2. One of the limitations of this approach is that for system (20), the argument of the trigonometric functions defined in (36) is \sqrt{C} , which is a square root of matrix C , i.e., $(\sqrt{C}) \cdot (\sqrt{C}) = C$. However, the authors in [1] approximate the action of trigonometric functions over vectors without actually computing \sqrt{C} . The algorithm is based on a truncated Taylor series and recurrences of Chebyshev polynomials. We have employed the code from [1] to compute the method defined in (36) for the numerical results in this work. This code also utilizes a dense matrix, although of one quarter of the size with respect to that employed in [8].

7. Numerical results

In the numerical results, we approximate (19) employing φ -functions as explained in Section 5.1. We verify the results by employing the two first MATLAB routines described in Section 6. We have also computed (36) with the last routine mentioned in Section 6. All algorithms deliver the same convergence results for the examples of this section. For 1D/2D + time wave equation, we employ a FEM with piecewise linear functions for the numerical discretization of the space variable.

Example 1: We consider the second order ODE (1) where the exact solution is

$$u(t) = c_1 \cos(\alpha t) + c_2 \sin(\alpha t),$$

where we set $\alpha = 18\pi$ and $I = [0, 1]$. Here, we have $f = 0$, $u_0 = c_1$ and $v_0 = c_2\alpha$. We also set $c_1 = 1$ and $c_2 = 0$. Figures 1 - 4 show the exact and the DPG solutions solving (19) for $p = 0, 1, 2, 3$. Figure 5 illustrates the convergence of the error for p up to 3 where we observe a convergence rate of $p + 1$. We obtain analogue results as in the DPG method for the 1D wave equation in frequency domain [38].

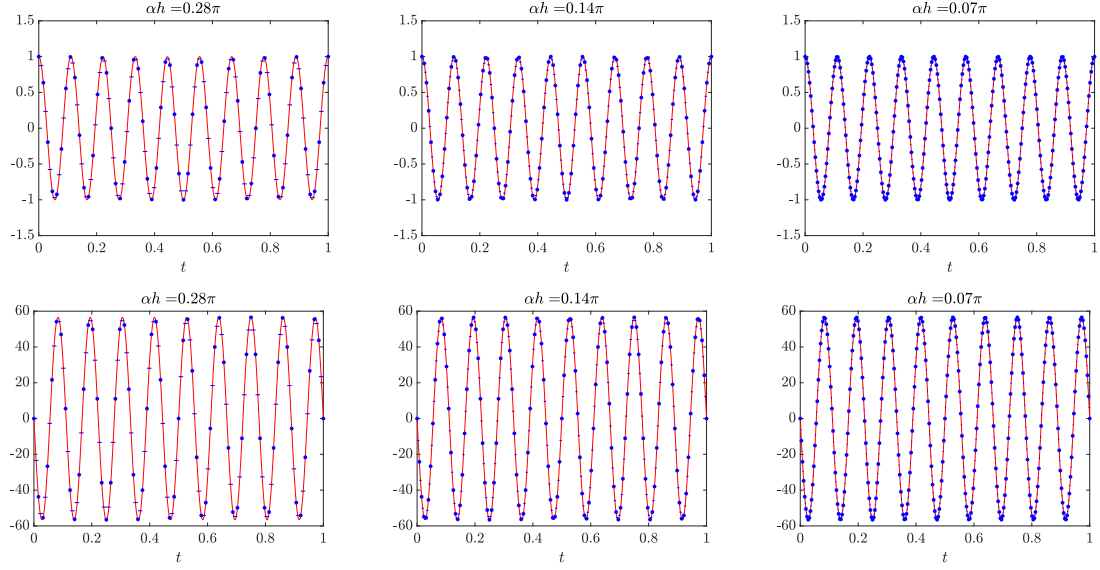


Figure 1: Approximated solution $u(t)$ (first row) and velocity $v(t)$ (second row) of Example 1 with $p = 0$.

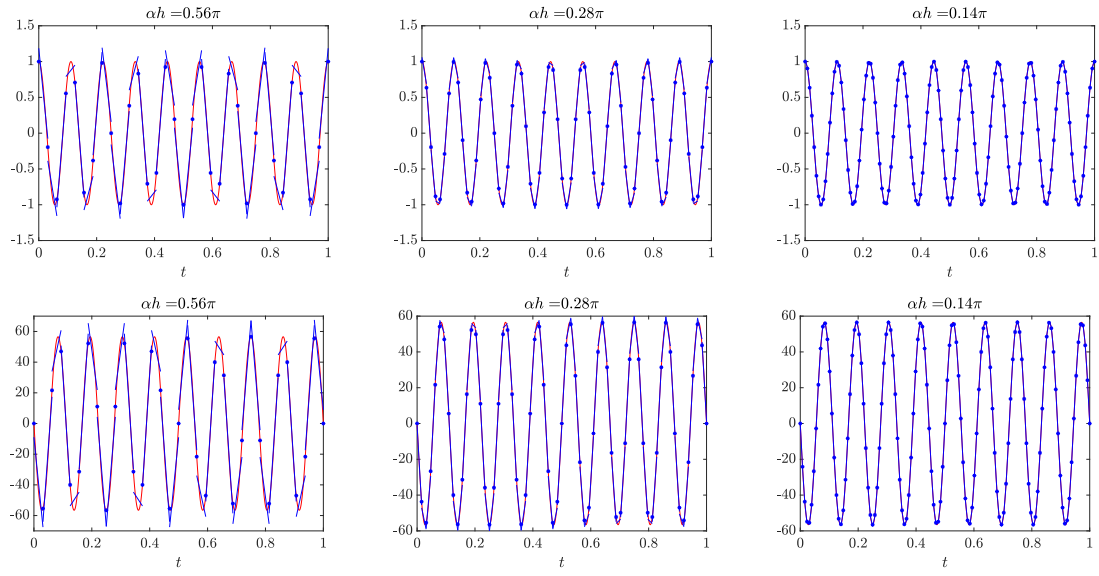


Figure 2: Approximated solution $u(t)$ (first row) and velocity $v(t)$ (second row) of Example 1 with $p = 1$.

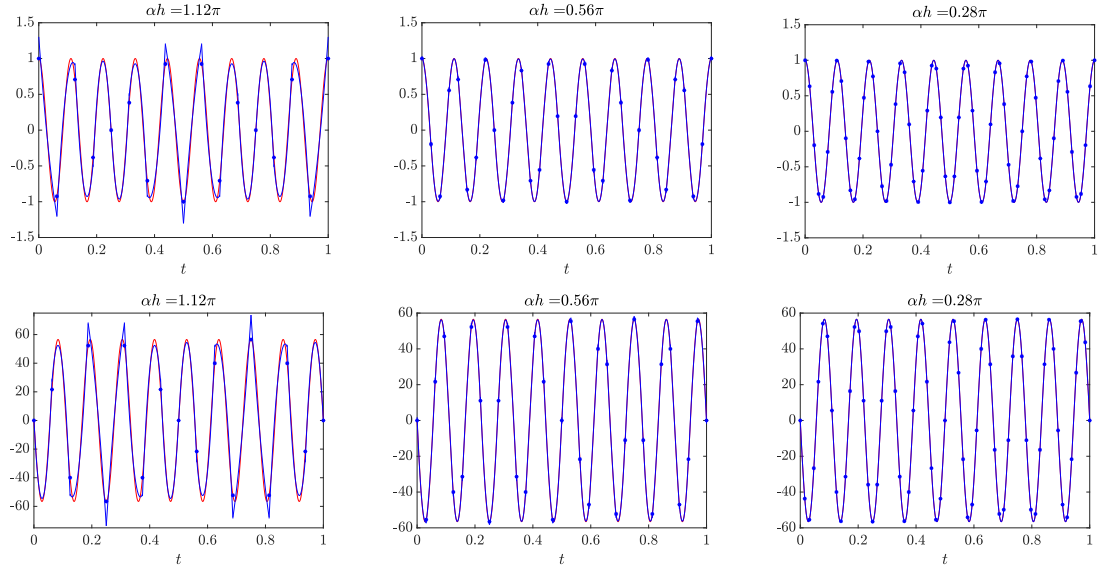


Figure 3: Approximated solution $u(t)$ (first row) and velocity $v(t)$ (second row) of Example 1 with $p = 2$.

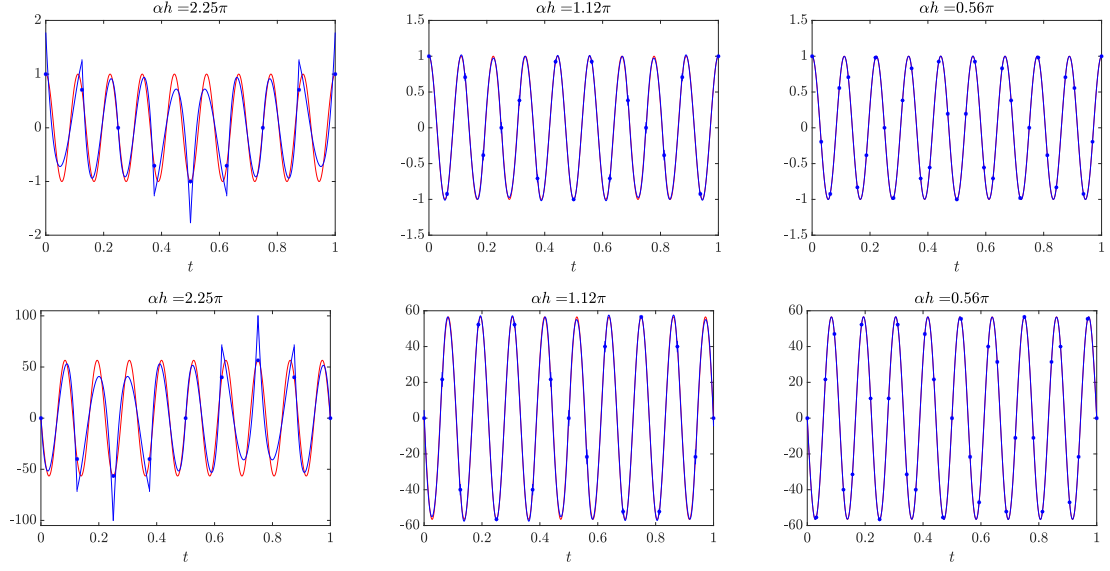


Figure 4: Approximated solution $u(t)$ (first row) and velocity $v(t)$ (second row) of Example 1 with $p = 3$.

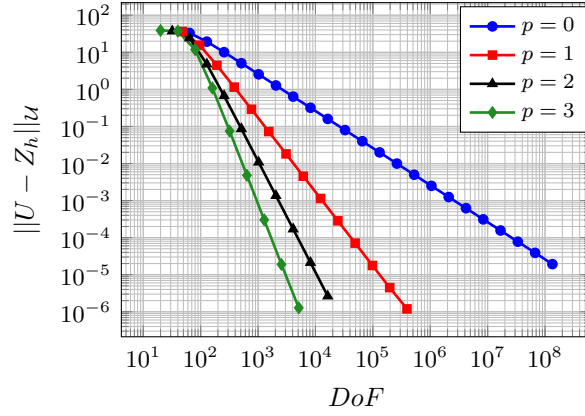


Figure 5: Convergence of the error for $p = 0, 1, 2, 3$ of Example 1.

Example 2: We now consider the 1D+time linear wave equation

$$\begin{cases} u_{tt} - (\alpha u_x)_x = f(x, t), & \forall (x, t) \in \Omega \times I, \\ u(x, t) = 0, & \forall (x, t) \in \partial\Omega \times I, \\ u(x, 0) = u_0(x), & \forall x \in \Omega, \\ u_t(x, 0) = v_0(x), & \forall x \in \Omega, \end{cases} \quad (39)$$

where the data is selected in such a way that the exact solution is

$$u(x, t) = \cos(\alpha_0 t) \sin(\alpha_1 x).$$

We set $\Omega = (0, 1)$, $I = (0, 1]$, $\alpha_0 = 14\pi$ and $\alpha_1 = 2\pi$. For the discretization in space we employ a FEM with piecewise linear functions and 10^3 elements. Figure 6 shows the approximated solutions and velocities for $p = 0, 1, 2$ with a fixed number of time steps. Figure 7 displays the relative error in % for $p = 0, 1, 2, 3$. We conclude that the error remains constant when the discretization error in space becomes dominant.

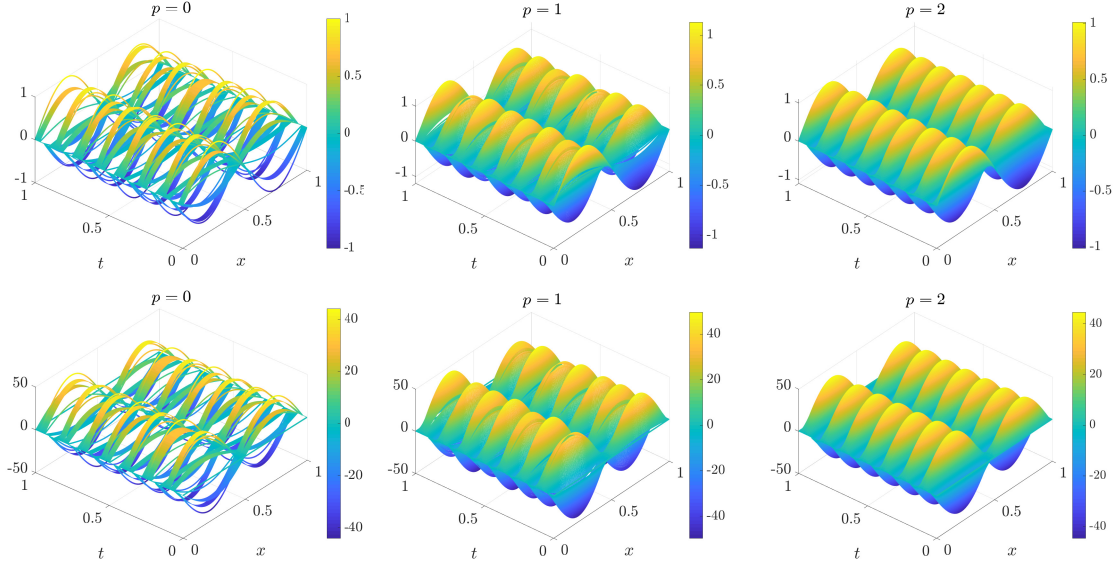


Figure 6: Approximated solution (top row) and derivative (bottom row) of Example 2 with 2^5 time steps.

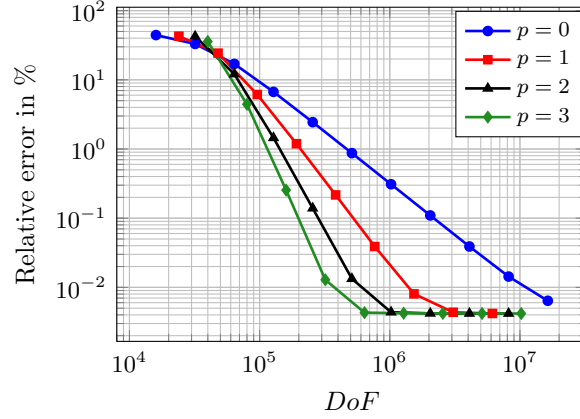


Figure 7: Convergence of the error for $p = 0, 1, 2, 3$ of Example 2.

Example 3: We consider a 1D+time example that is similar to the one considered in [26]. In (39), we set $\Omega = (0, 1)$ and $I = (0, 1.5]$, and we select $f(x, t) = 0$,

$$\alpha(x) = \begin{cases} 2, & \text{if } x < 1/2, \\ 1/2, & \text{if } x \geq 1/2, \end{cases}$$

and the initial conditions

$$u(x) = e^{-250(x-0.25)^2}, \quad v(x) = 0.$$

Figure (8) shows the approximations of $u(x, t)$ and $v(x, t)$ for $p = 0, 1, 2, 3$ for a fixed number of 2^5 time steps and 500 elements in space.

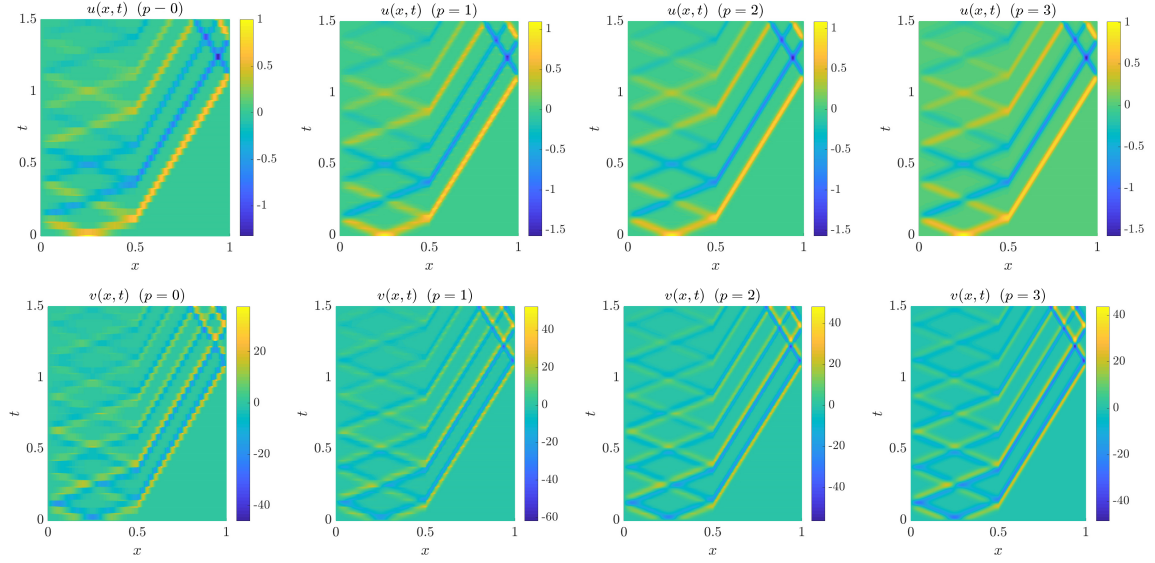


Figure 8: Approximated solution of $u(x, y)$ (top row) and $v(x, t)$ (bottom row) of Example 3 for $p = 0, 1, 2, 3$ and 2^5 time steps.

Example 4: We consider a 2D+time example similar to one shown in [6]

$$\begin{cases} u_{tt} - \nabla \cdot (\alpha \nabla u) = f(x, y, t), & \forall (x, y, t) \in \Omega \times I, \\ u(x, y, t) = 0, & \forall (x, y, t) \in \partial\Omega \times I, \\ u(x, y, 0) = u_0(x, y), & \forall (x, y) \in \Omega, \\ u_t(x, y, 0) = v_0(x, y), & \forall (x, y) \in \Omega, \end{cases} \quad (40)$$

where $\Omega = (-0.5, 0.5)^2$ and $I = (0, 1]$. We set a discontinuous wave speed

$$\alpha(x, y) = \begin{cases} 1, & \text{if } y < 1/8, \\ 8, & \text{if } y \geq 1/8, \end{cases}$$

$f(x, y, t) = 0$, and the initial conditions

$$u_0(x, y) = e^{-|\mathbf{x}_s|^2} (1 - |\mathbf{x}_s|^2) \Theta(1 - |\mathbf{x}_s|), \quad v_0(x, y) = 0,$$

where $|\mathbf{x}_s| = (x/s)^2 + (y/s)^2$ with $s = 0.05$, and the jump function symbol is given by

$$\Theta(x, y) = \begin{cases} 0, & \text{if } x < 0, \\ 1, & \text{if } x \geq 0. \end{cases}$$

For the discretization in space, we select a mesh of 128×128 elements and we perform mass lumping [29] to obtain a diagonal mass matrix. We select 2^4 time steps and piecewise constant functions in time. Figure 9 shows the colormap of the solution in the element interiors in time at different time steps.

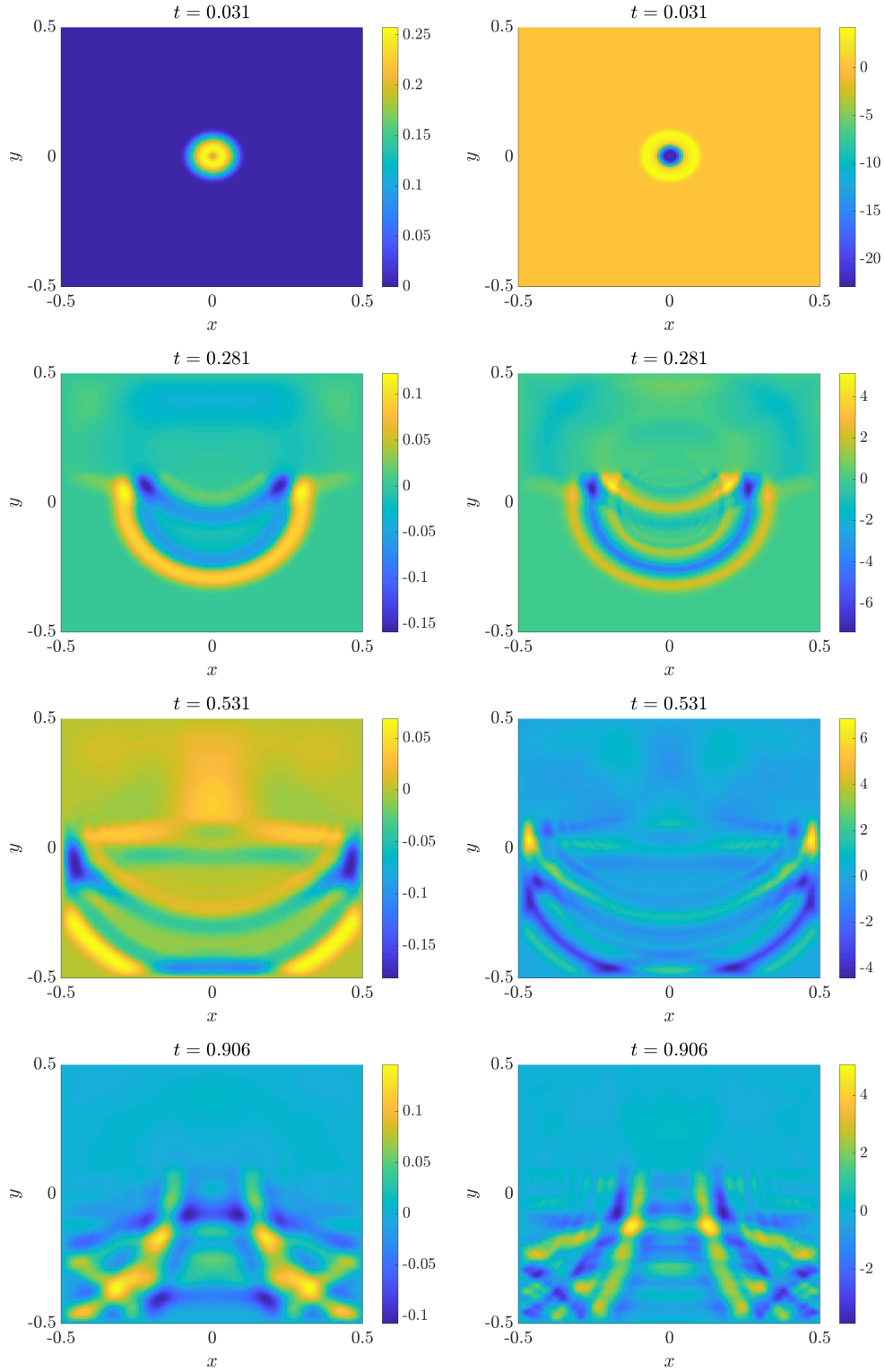


Figure 9: Approximated interior solution of $u(x,y,t)$ (left column) and $v(x,y,t)$ (right column) of Example 4 for $p = 0$ at different times.

8. Conclusions

We extend our previous work [35] on DPG-based time integrators for linear parabolic PDEs to hyperbolic problems. We first reduce the second-order equation to a first order system in time by introducing the velocity $v = u_t$. This doubles the system size compared to the parabolic case. Then, we calculate the optimal test functions analytically and we obtain exponentials of the operator in space. We relate our method to exponential integrators using either φ -functions or trigonometric functions. We discuss different existing routines for the approximation of such functions and the computational limitations comparing with the parabolic case. Finally, we numerically show the performance of our method employing both φ -functions and trigonometric functions to compute the optimal testing. In space, we employ a FEM. For the 2D+time example, we perform mass lumping to obtain a diagonal mass matrix. In all cases, we obtain $p + 1$ convergence order for uniform refinements in time.

Possible future work includes: (a) to extend the proposed DPG method in time to transient nonlinear PDEs; (b) to combine both DPG in space together with DPG-based time-marching scheme; (c) to perform time adaptivity based on the error representation function from DPG; (d) to design different (goal-oriented) adaptive strategies; (e) to improve the iterative methods to approximate φ -functions for hyperbolic problems.

Appendix A. Cayley-Hamilton theorem

We consider a square matrix A of dimension n . The characteristic polynomial of A is defined as

$$P(s) = \det(sI_n - A) = \sum_{i=0}^n c_i s^i,$$

and we know that $p(\lambda_i) = 0, \forall i = 1, \dots, n$, where λ_i are the eigenvalues of A .

Similarly, we define the following matrix polynomial

$$P(X) = \sum_{i=0}^n c_i X^i,$$

where X is an arbitrary matrix of size n and $X^0 = I_n$. The Cayley-Hamilton theorem states that $P(A) = 0$.

We can use this result to express a matrix function $f(A)$ as a finite matrix polynomial. First, we assume that the scalar function $f(s)$ has the following series expansion

$$f(s) = \sum_{k=0}^{\infty} \beta_k s^k.$$

We can express $f(s)$ as

$$f(s) = Q(s)P(s) + R(s),$$

where $P(s)$ is the characteristic polynomial of A and $R(s)$ is a polynomial of order $n - 1$. From the Cayley-Hamilton theorem, as $P(A) = 0$, we have that

$$f(A) = R(A) = \sum_{k=0}^{n-1} \alpha_k A^k,$$

and we compute the coefficients α_k employing the eigenvalues of A

$$f(\lambda_i) = R(\lambda_i) = \sum_{k=0}^{n-1} \alpha_k \lambda_i^k, \quad \forall i = 1, \dots, n.$$

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